Supporting Information

Anisotropic Impact Sensitivity and Shock Induced Plasticity of TKX-50 (dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate) Single Crystals: From Large-Scale Molecular-dynamics Simulations

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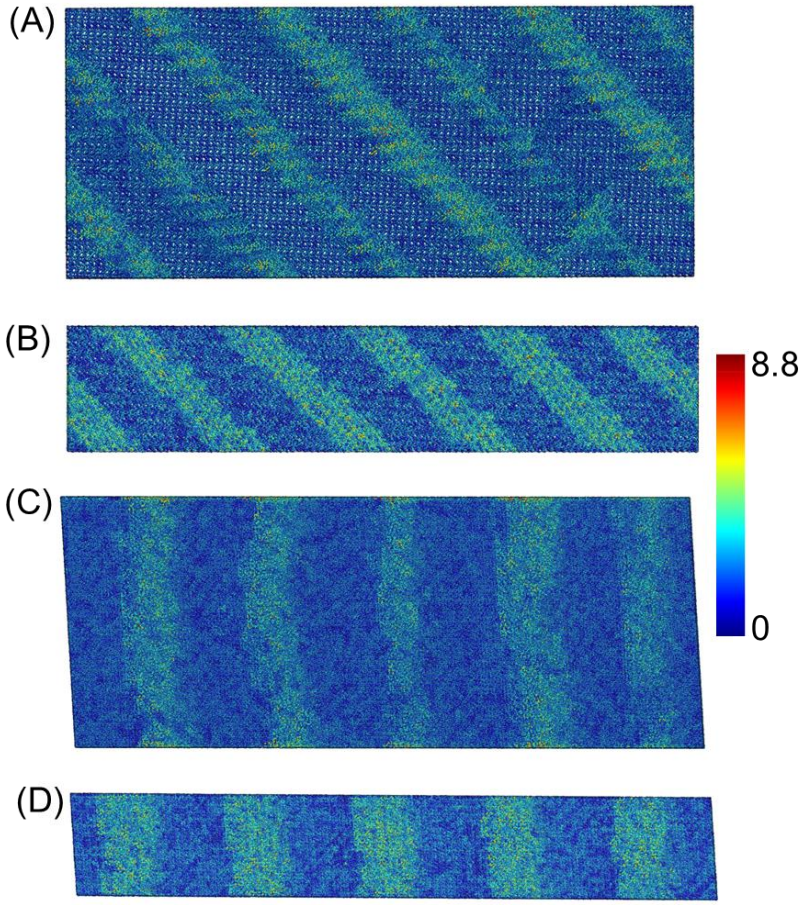

Figure S1. (A)-(D) Snapshots showing the plastic deformation in single crystal TKX-50 shock loaded along [100] direction with P_{xx} = 8.17 GPa. (A) Big cross section (19.4 × 18.0 nm^2) viewed along (001); (B) small cross section (9.7 × 9.0 nm^2) viewed along (001); (C) big cross section viewed along (010); (D) small cross section viewed along (010). Colors coding refers to MRD in Å.

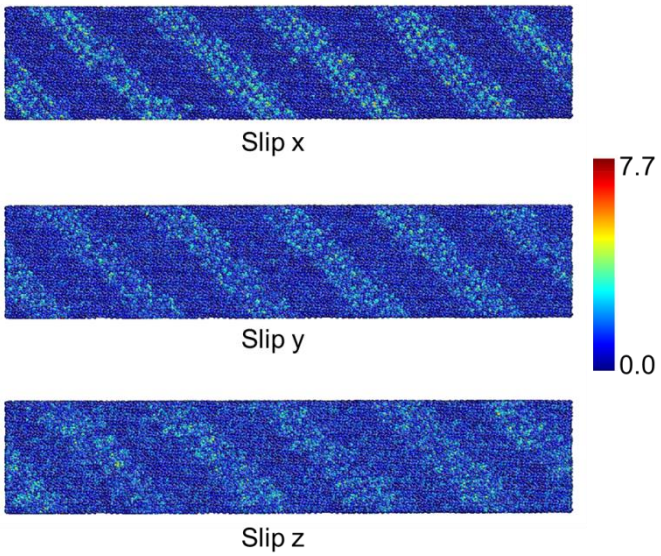

Figure S2. The MRDs of three directions for the [100] shock with Pxx = 8.17 GPa.

Force field parameters

Table S1: Equivalence table: AAT - apparent atom type; NB – nonbond; ATC - atom type charge; BINC - bond increment; A/C - angle center atom; A/S - angle side atom; T/C - torsion center atoms; T/S - torsion side atoms; O/C - out-of-plane center atom; O/S - out-of-plane side atoms

#AAT	NONB	ATC	BINC	BOND	A/C	A/S	T/C	T/S	O/C	O/S
c_35	c_35a	c_3a	c_3a	c_3a	c_35a	c_3a	c_3a	c_3a	c_3a	c_3a
c_35a	c_35a	c_3a	c_3a	c_3a	c_35a	c_3a	c_3a	c_3a	c_3a	c_3a
h_1n	h_1n	h_1n	h_1n	h_1n	h_1n	h_1n	h_1n	h_1n	h_1n	h_1n
h_1o	h_1o	h_1o	h_1o	h_1o	h_1o	h_1o	h_1o	h_1o	h_1o	h_1o
n_25	n_25a	n_2a	n_2a	n_2a	n_25a	n_2a	n_2a	n_2a	n_2a	n_2a
n_25a	n_25a	n_2a	n_2a	n_2a	n_25a	n_2a	n_2a	n_2a	n_2a	n_2a
n_25b	n_25a	n_25b	n_25b	n_25b	n_25b	n_2a	n_2a	n_25b	n_2a	n_2a
n_25c	n_25c	n_25b	n_25b	n_25b	n_25b	n_2a	n_2a	n_25b	n_2a	n_2a
n_3	n_35a	n_3a	n_3a	n_3a	n_35a	n_3a	n_3a	n_3a	n_3a	n_3a
n_35+	n_35a	n_3a	n_3a	n_3a	n_35a	n_3a	n_3a	n_3a	n_3a	n_3a
n_35a	n_35a	n_3a	n_3a	n_3a	n_35a	n_3a	n_3a	n_3a	n_3a	n_3a
n_3h2	n_3h2	n_3h2	n_3	n_3	n_3	n_3	n_3	n_3	n_3	n_3
n_4+	n_3h2	n_4+	n_3	n_3	n_3	n_3	n_3	n_3	n_3	n_3
n_4o	n_3h2	n_4+	n_3	n_3	n_3	n_3	n_3	n_3	n_3	n_3
o_1	o_1	o_1	o_1	o_2	o_2	o_2	o_2	o_2	o_2	o_2
o_2	o_2	o_2	o_2	o_2	o_2	o_2	o_2	o_2	o_2	o_2

Table S2. Bond stretch parameters

i	j	r_0 (Å)	K_r (kcal/mol)
c_3a	c_3a	1.4449	423.1528
c_3a	n_25b	1.33	472.3025
c_3a	n_2a	1.33	447.6915
c_3a	n_3a	1.34	412.2653
h_1n	n_3	1.0172	482.9013
h_1o	o_2	0.9601	607.7293
n_25b	n_2a	1.4068	170.1522
n_2a	n_2a	1.3343	391.9421
n_2a	n_3a	1.3301	282.6883
n_3	o_2	1.415	250.3399
n_3a	o_2	1.3081	429.293

Table S3. Angle Parameters

i	j	k	Θ_0 (degree)	K_Θ(kcal/mol)
c_3a	c_35a	n_2a	114.6366	10
c_3a	c_35a	n_3a	112.2974	10
c_3a	n_25a	n_2a	116.3865	81.0226
c_3a	n_25b	n_2a	116.3865	169.4014
c_3a	n_35a	n_2a	120.2883	10
c_3a	n_35a	o_2	116.3429	70.3832
h_1n	n_3	h_1n	104.4437	45.0197
h_1n	n_3	o_2	102.2616	40.1935
h_1o	o_2	n_3	98.1158	30.9061
h_1o	o_2	n_3a	100.2234	47.4074
n_2a	c_35a	n_3a	118.6362	67.3488
n_2a	n_25a	n_2a	122.1918	190.7093
n_2a	n_25a	n_3a	116.4971	130.3387
n_2a	n_35a	o_2	109.2394	56.2987

Table S4. Torsion angle parameters

i	j	k	l	Y (degree)	V_n (kcal/mol)	n
c_3a	c_3a	n_2a	n_2a	180	9.0435	2
c_3a	c_3a	n_3a	n_2a	180	3.2989	2
c_3a	c_3a	n_3a	o_2	180	1.8858	2
c_3a	n_2a	n_2a	n_2a	180	4.1548	2
c_3a	n_3a	n_2a	n_2a	180	10.2354	2
c_3a	n_3a	o_2	h_1o	180	0.2574	2
h_1n	n_3	o_2	h_1o	180	-2.5896	2
h_1o	o_2	n_3a	n_2a	180	0.6048	2
n_25b	c_3a	c_3a	n_25b	180	4.3784	1
n_25b	c_3a	c_3a	n_3a	180	5.3257	1
n_25b	c_3a	n_3a	n_2a	180	-3.6033	2
n_25b	c_3a	n_3a	o_2	180	5.4451	2
n_25b	n_2a	n_2a	n_3a	180	8.4242	2
n_2a	c_3a	c_3a	n_2a	180	3.534	2
n_2a	c_3a	c_3a	n_3a	180	3.4204	2
n_2a	c_3a	n_3a	n_2a	180	24.1859	2
n_2a	c_3a	n_3a	o_2	180	8.7998	2
n_2a	n_2a	c_3a	n_3a	180	2.8434	2
n_2a	n_2a	n_2a	n_3a	180	21.344	2
n_2a	n_2a	n_3a	o_2	180	5.4309	2
n_3a	c_3a	c_3a	n_3a	180	1.1264	2

Table S5. Improper Torsion

i	j	k	l	X_0 (degree)	K_X(kcal/mol)	n
c_3a	n_2a	c_3a	n_3a	180	5.01	2
c_3a	n_2a	n_3a	o_2	180	5	2
h_1n	h_1n	n_3	o_2	0	0.8362	3